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Progress is reported on research in molecular physics involving electron-bombardment molecular dissociation. The velocity distribution of metastable and ionic fragments are measured using a pulsed electron beam and a time-of-flight technique. Fragments from the hydrogen molecule and its deuterated forms have been investigated using electron energies from 30 to 100 electron-volts. Dissociation channels via particular molecular or molecular ion excited states have been proposed to explain observed features in the velocity spectra

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A similar experiment involving hydrogen fragments from the hydrogen halides is also in progress. Preliminary data show several resolved velocity groups indicating the presence of multiple dissociating channels. Experiments using water and hydrogen sulfide molecules are also underway. Finally, we are continuing to develop our ion mass filter which allows us to obtain separate ion velocity distributions for each mass in a situation in which several ion masses are present.

Annual Technical Report

"Time-of-Flight Spectroscopy of Molecular Structure, Collision Processes, and Gas-Surface Interactions"

Principal Investigators

Willis E. Lamb, Jr., Professor of Physics and Optical Sciences

L. C. McIntyre, Jr., Professor of Physics

AFOSR 80-0218

Summary of research June 1980 - June 1981

Research sponsored by the Air Force Office of Scientific Research, Air Force Systems Command, United States Air Force.

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July 15, 1981

CONTENTS

I. Research Status

A. Introduction

This report contains a summary of research in molecular physics conducted under AFOSR grant 80-0218 during the period 15 June 1980 to 14 June 1981. The research was done in the Department of Physics at the University of Arizona by faculty and staff of the Department of Physics and the Optical Sciences Center. The major objectives stated in our proposal for this contract period were:

1. A study of H(2S) and H^+ fragments from the dissociation of H_2 .
2. A study of H(2S) fragments from the dissociation of HCl.
3. A study of H(2S) fragments from the dissociation of H_2O.

Item 1 represents the continuation of a series of experiments involving the hydrogen molecule which has occupied this laboratory for some time. This work has resulted in two publications during the year and included measurements on D_2 and HD as well as on H_2 . The other two experiments are still in progress and have been expanded to include both H(2S) and H^+ fragments. Considerable effort was made during this period to improve our experimental techniques, mainly in the area of electron gun design.

Our experiments consist of time-of-flight measurements of metastable and ionic fragments resulting from electron bombardment dissociation of molecules. The electron beam is pulsed and intersects a beam of molecules, some of which dissociate producing fragments with a few eV kinetic energy. The fragments traverse a path of approximately 20 cm in a direction perpendicular to both the electron and molecular beams and are then detected. A velocity spectrum is accumulated by measuring the distribution of time intervals between an electron beam pulse and a fragment detection. In some cases, information on repulsive states of the excited molecule can be inferred from the velocity distribution of the fragments. Details of specific experiments are given in the following paragraphs.

B . Ionic fragments from dissociation of H_2, D_2 , and HD.

Kinetic energy distributions of ion fragments from electron bombardment dissociated H_2, D_2, and HD were measured at electron energies between 30 and 100 eV. All measurements were made at 90 degrees relative to the electron beam. The threshold for H^+ production is about 18 eV corresponding to excitation of H_2^+ to the repulsive portion of its ground state potential energy curve. These ion fragments have a kinetic energy distribution ranging from zero to a few tenths of an eV. We do not observe these fragments. The next onset involving H_2^+ states is at about 29 eV where the repulsive $^2\Sigma_u^+$ state yields H^+ fragments with kinetic energies centered at about 8.5 eV. At an observation angle of 55 degrees this is the dominant process; however, at least near threshold, selection rules first stated by Dunn predict that the angular distribution of H^+ fragments from this $^2\Sigma_u^+$ state have a $\cos^2\theta$ dependence and therefore should have no yield at 90 degrees . This appears to be the case, since in our experiment we were able to postulate dissociation channels to explain the observed data without participation of this channel.

Another source of H^+ fragments in this experiment, in addition to the many higher states of H_2^+ , is autoionizing excited states of H_2. Several such known states were considered, however our data below 50 eV bombarding energy was fitted assuming contributions from only two autoionizing states ($^1\Sigma_g^+$ and $^1\pi_u$) and one repulsive state of H_2^+ ($^2\pi_u$). The shapes of the kinetic energy distributions for H^+ from H_2 and D^+ from D_2 are substantially different, and a strong preference for H^+ over D^+ fragments from HD was observed. Further details concerning this experiment can be found in our paper published in the June 1980 issue of Physical Review A.

C. H(2S) and D(2S) fragments from H_2 and D_2

We give here the abstract of our paper published in the November 1980 issue of Physical Review A.

Time-of-flight spectra of H(2S) and D(2S) fragments from electron-bombardment dissociated H_2 and D_2 have been observed. Kinetic energy distributions of "fast" metastable fragments were obtained for electron-bombardment energies ranging from near the threshold for fast metastable production (less than 29 eV) to 100 eV. At low bombarding energies previously unreported structure is observed in the fast peaks for both isotopes. At high bombarding energies also there is evidence of unresolved structure in the fast peaks. The present data are compared with the results of earlier investigations. At low bombarding energies there are significant discrepancies between the present results and previous measurements. At high bombarding energies there is significant disagreement with a calculation that assumes a single dissociating state. The observed shift of the fast peak as a function of the bombarding electron energy is compared to predictions incorporating a form of the Wannier law. This comparison tends to confirm the presence of more than one dissociation channel yielding fast metastables. Several excited states of H_2 and H_2^+ are discussed as possible channels contributing to the observed kinetic energy distributions.

D. H(2S) and H^+ fragments from hydrogen halides

Our proposed experiment on H(2S) fragments from HCl has been expanded to include HBr, HI, and HF as well as observation of H^+ fragment kinetic energy distributions. Our initial H^+ kinetic energy distributions show several distinguishable features in each species indicating multiple dissociation channels. We have spent considerable effort during the year developing electron guns with better energy resolution in order to accurately determine the appearance potential of these features. The electron gun we normally use contains a resistively heated 1-mil tungsten wire 2 cm long which has about 2 volts potential difference between the ends resulting in a 2 eV spread in electron energy. We are experimenting with two methods to reduce this spread; one involving the use of a hairpin shaped filament which emits electrons from a small portion of the wire filament, the other involving an indirected heated emitter.

E. H(2S) and H^+ fragments from H_2O

In addition to the preliminary data on H(2S) fragments from dissociated H_2O presented in our proposal we have taken some data on the H^+ ion spectra from this molecule. This experiment is still in progress and our plans include a search for H_2^+ fragments using our mass filter and extension to include dissociation of H_2S molecules.

II. Personnel

We list below personnel associated with this research program:

Principal investigators:

W. E Lamb Jr.

B.S. (Chemistry) University of California (Berkeley) 1934

Ph.D. (Physics) University of California (Berkeley) 1934

D.Sc. University of Pennsylvania 1953

M.A. (by decree) Oxford University 1956

M.A. (hon.) Yale University 1961

L.H.D. Yeshiva University 1965

D.Sc. Gustavus Adolphus College 1975

L. C. McIntyre Jr.

B.S. (Physics) Stanford University 1957

M.S. (Physics) University of Wisconsin 1961

Ph.D. (Physics) University of Wisconsin 1965

Research Associate:

Otto F. Kalman

B.S. (Chemical Engineering) Purdue University 1955

Ph.D. (Physical Chemistry) Princeton University 1959

Research Assistants:

Richard Cordaro

B.A. Millersville St. College, Penn. 1973

M.S. (Physics) Lehigh University 1978

Bruce Kittams

B.S. Oregon State University 1971

M.S. (Physics) University of Arizona 1981

Joseph Spezeski, a Research Associate during part of the preceeding year, left in March to take a position with Hughes Aircraft in Tucson.

III. Publications

1. M. D. Burrows, L. C. McIntyre, Jr., S. R. Ryan, and W. E. Lamb, Jr., "Dissociative ionization of H_2, D_2, and HD using electron-impact excitation," Phys. Rev. A 21, 1841 (1980).

2. J. J. Spezeski, O. F. Kalman, and L. C. McIntyre, Jr., "Time-of-fight study of H(2S) and D(2S) produced by electron impact on H_2 and D_2: Fast Peaks," Phys. Rev. A 22, 1906 (1980).


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